Molecular dynamics investigations of the strengthening of Al-Cu alloys during thermal ageing

Aluminium is, next to iron, one of the most widely used metals in engineering. However, in its pure form it has rather poor material properties. By adding various other elements such as e.g. Cu, Mn, Zn, and/or Si, it is possible to enhance its mechanical properties, depending on the type of the alloying material and the thermal ageing state.

The ageing process of an Al-Cu alloy can be classified into five distinct stages. At the first stage, a supersaturated solid solution is present, with substitutionally disolved copper atoms embedded in the aluminium matrix. In the binary Al-Cu material system the precipitate formation results in coherent single layer Cu-discs, known as Guinier-Preston(GP) zones. GP zones generally occupy {100} crystallographic planes, their diameter reaches up to 10 nm. In the subsequent ageing state of Al-Cu alloys, further Cu-discs are formed in the vicinity of the existing ones. This results in the formation of GP II zones. The internal structure of a GP II zone consists of several GP I zones parallel to each other, in between which several Al-layers are found.

Classical molecular dynamics simulations of the interaction of edge dislocations with solid soluted copper atoms and Guinier-Preston zones in aluminium are performed using EAM potentials. Critical resolved shear stresses (CRSSs) are calculated for different concentrations of solid soluted copper. In case of precipitate strengthening, the GP zone size, its orientation and offset from the dislocation plane are taken as simulation parameters. It is found that in case of solid soluted copper, the CRSS is proportional to the copper concentration. In case of the two subsequent aging stages both the dislocation depinning mechanism as well as the depinning stress is highly dependent on the GP zone orientation and to a lesser degree to its size.

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